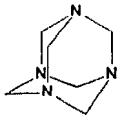
PubChem
Information on biological activities of small molecules

Compound Summary:



CID: 4101

BioActivity: Summary
Inactive: 10 Links
Inconclusive: 1 Link

NLM Toxicology:
Link1, Link2

Substances:
All: 144 Links
Same: 39 Links
Mixture: 105 Links

Related Compounds:
Same, Connectivity: 3 Links

Similar Compounds: 18 Links

Structure Search

MeSH | Synonyms | Properties | Descriptors | Category | Exports

Medical Subject Annotations: (Total:1)

Methenamine
An anti-infective agent most commonly used in the treatment of urinary tract infections. Its anti-infective action derives from the slow release of formaldehyde by hydrolysis at acidic pH. (From Martindale, The Extra Pharmacopoeia, 30th ed, p173)

Show MeSH Tree Structure

Pharmacological Action:
Anti-Infective Agents, Urinary

PubMed via MeSH Choose by Subheadings:

administration and dosage	adverse effects	analogs and derivatives
analysis	blood	chemical synthesis
chemistry	diagnostic use	economics
immunology	metabolism	pharmacokinetics
pharmacology	poisoning	standards
therapeutic use	therapy	toxicity
urine		

PubMed MeSH Keyword Summary

Depositor-Supplied Synonyms: (Total: 123)

Display: First 10 | All | Sort: Weight

methenamine
Hexamine
Urotropin
Urotropine
Uritone
Hexamethylenetetramine
Antihydral
Methenamin
Resotropin
Aminoform
Ammoform
Cystamin
Cystogen
Duirexol
Formamine
Hexaform
Hexaloids
Uratrine
Urodeine
Xametrin

Heterin
Hexasan
Formin
Uramin
Aminoformaldehyde
Hexamethylenamine
Preparation AF
Mandelamine
Hexamethyleneamine
Hexaminum
Hexilmethylenamine
Methamin
Metramine
Hexa-Flo-Pulver
Ekagom H
Ammonioformaldehyde
Uro-phosphate
Aceto HMT
Herax UTS
Hexamethylentetramin
Nocceler H
Sanceler H
Formin (heterocycle)
Prestwick_79
Hexamethylenetetraamine
Hexamine (JAN)
Hexamine (TN)
Hexamethylene tetramine
Hexamethylentetramine
Hexasan (VAN)
Hexamine (heterocycle)
Methenamine (USP)
Vulkacit H 30
1,3,5,7-Tetraazaadamantane
Hexamethylentetraminum
HMTA
S 4 (heterocycle)
Hexamethylenetetraminum
Caswell No. 482
Spectrum_000991
Spectrum2_000827
Spectrum3_001730
Spectrum4_000872
Methenamine [USAN:INN]
component of Uro-Phosphate
Metenamina [INN-Spanish]
Methenaminum [INN-Latin]
Esametilentetramina [Italian]
H11300_ALDRICH

Hexamethylenetetramine, tech.
Hexamethylentetramin [German]
KBioGR_001563
KBioSS_001471
DivK1c_000322
SPECTRUM1500394
SPBio_000753
Hexamethylenetetramine solutions
15614_RIEDEL
33233_RIEDEL
CCRIS 2297
CHEBI:6824
H6404_SIAL
HSDB 563
Hexa (vulcanization accelerator)
NSC26346
KBio1_000322
KBio2_001471
KBio2_004039
KBio2_006607
KBio3_002600
NINDS_000322
NSC403347
AIDS018490
Formin (the heterocyclic compound)
398160_SIAL
AIDS-018490
EINECS 202-905-8
EINECS 246-528-7
NSC 26346
UN1328
EPA Pesticide Chemical Code 045501
NSC 403347
100-97-0
AI3-09611
1,3,5,7-tetraazatricyclo[3.3.1.1~3,7~]decane
D00393
Hexamethylenetetramine-palladium chloride adduct
1,3,5,7-Tetraazatricyclo(3.3.1.13,7)decane
1,3,5,7-Tetraazatricyclo[3.3.1.13,7]decane
1,3,5, 7-Tetraazatricyclo[3.3.1.13,7]decane
1,3,5,7-Tetraazatricyclo[3.3.1.1(3,7)]decane
Hexamethylenetetramine [UN1328] [Flammable solid]
1,3,5,7-Tetraazatricyclo (3.3.1.1(3,7))decane
1,3,5,7-Tetraazatricyclo(3.3.1.1(sup 37))decane
1,3,5,7-Tetraazatricyclo(3.3.1.13,7)decane hydroiodide
HMT
InChI=1/C6H12N4/c1-7-2-9-4-8(1)5-10(3-7)6-9/h1-6H
11103-67-6

15978-33-3
24911-88-4
56549-34-9
74734-16-0
91773-48-7

Properties Computed from Structure:

Molecular Weight: 140.18628 g/mol
Molecular Formula: $C_6H_{12}N_4$
Hydrogen Bond Donor Count: 0
Hydrogen Bond Acceptor Count: 4
Rotatable Bond Count: 0
Topological Polar Surface Area: 13
more...

Descriptors Computed from Structure:

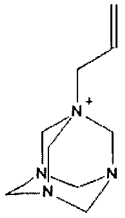
Canonical SMILES: C1N2CN3CN1CN(C2)C3
InChI: InChI=1/C6H12N4/c1-7-2-9-4-8(1)5-10(3-7)6-9/h1-6H2

Substance Category:

Biological Properties: 22 Links
Journal Publishers: 1 Link
Metabolic Pathways: 1 Link
Molecular Libraries Screening Center Network: 2 Links
Physical Properties: 4 Links
Substance Vendors: 6 Links
Theoretical Properties: 1 Link
Toxicology: 3 Links

ASN1	Display	XML	Display	SDF	Display
	Save		Save		Save

Compound Summary:



CID: 407405

BioActivity: Summary
Active: 7 Links
Inactive: 66 Links

NLM Toxicology: Link

Substances:
All: 9 Links
Same: 6 Links
Mixture: 3 Links

Similar Compounds: 5 Links

Structure Search

Synonyms | Properties | Descriptors | Category | Exports

Depositor-Supplied Synonyms: (Total: 17)

Display: First 10 | All | Sort: Weight

Allyliodourotropine
Allyl iodide hexamine
Methenamine allyl iodide
Methenamine allyloiodide
CBDivE_014100
Iodoallylhexamethylenetetramine
Hexamethylenetetramine alliodide
NSC5062
NSC7309
Allyl iodide hexamethylenetetramine
Hexamethylenetetramine allyl iodide
EINECS 253-259-9
NCI60_004218
Hexamethylenetetramine, compd. with 3-iodopropene (1:1)
Propene, 3-iodo-, compd. with hexamethylenetetramine (1:1)
36895-62-2
3,5, 7-Triaza-1-azoniatricyclo[3.3.1.13,7]decane, 1- (2-propenyl)-, iodide

Properties Computed from Structure:

Molecular Weight: 181.25808 g/mol
Molecular Formula: $C_9H_{17}N_4^+$
Hydrogen Bond Donor Count: 0
Hydrogen Bond Acceptor Count: 3
Rotatable Bond Count: 2
Topological Polar Surface Area: 9.7
more...

Descriptors Computed from Structure:

Canonical SMILES: C=CC[N+]12CN3CN(C1)CN(C3)C2
InChI: InChI=1/C9H17N4/c1-2-3-13-7-10-4-11(8-13)6-12(5-10)9-13/h2H,1,3-9H2/q+1

Substance Category:

Biological Properties: 4 Links
Theoretical Properties: 1 Link
Toxicology: 1 Link

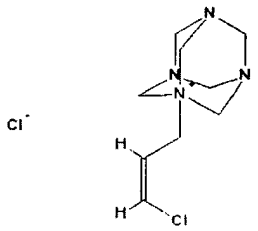
ASN1	Display	Save	XML	Display	Save	SDF	Display	Save

NCBI

PubChem

Information on biological activities of small molecules

Compound Summary:



CID: 6435993

Parent CID: 5346454
Unique Components: 2 Links

NLM Toxicology: Link

Substances: 3 Links

Related Compounds:
Same, Connectivity: 2 Links

Similar Compounds: 11 Links

Structure Search

Synonyms | Properties | Descriptors | Category

Depositor-Supplied Synonyms: (Total: 7)

Sort: Weig

Dowicil 200
Chloroallyl methenamine chloride
Hexamethylenetetramine chloroallyl chloride, cis isomer
1-(3-Chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride, cis form
3,5,7-Triaza-1-azoniatricyclo(3.3.1.13,7)decane, 1-((2Z)-3-chloro-2-propenyl)-, chloride
3,5,7-Triaza-1-azoniatricyclo(3.3.1.13,7)decane, 1-(3-chloro-2-propenyl)-, chloride, (Z)-
51229-78-8

Properties Computed from Structure:

Molecular Weight: 251.15614 g/mol
Molecular Formula: $C_9H_{15}Cl_2N_4$
Hydrogen Bond Donor Count: 0
Hydrogen Bond Acceptor Count: 4
Rotatable Bond Count: 2
Topological Polar Surface Area: 9.7
more...

Descriptors Computed from Structure:

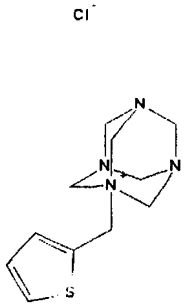
Canonical SMILES: C1N2CN3CN1C[N+](C2)(C3)CC=CCl.[Cl-]
Isomeric SMILES: C1N2CN3CN1C[N+](C2)(C3)C\C=C/Cl.[Cl-]
InChI: InChI=1/C9H16ClN4.ClH/c10-2-1-3-14-7-11-4-12(8-14)6-13(5-11)9-14;/h1-2H,3-9H2;1H/q+1;/p-1/b2-1-;/fC9H16C

Substance Category:

Biological Properties: 1 Link
Journal Publishers: 1 Link
Toxicology: 1 Link

ASN1 Display Save | XML Display Save | SI

Compound Summary:



CID: 22730
Parent CID: 22731
Unique Components: 2 Links

NLM Toxicology: Link

Substances: 3 Links

Similar Compounds: 3 Links

Structure Search

Synonyms | Properties | Descriptors | Category | Exports

Depositor-Supplied Synonyms: (Total: 8)

Sort: Weight

NSC49660
NSC 30209
NSC 49660

1-(2-Thenyl)hexamethylenetetrammonium chloride
HEXAMETHYLENETETRAMINIUM, 1-(2-THENYL)-, CHLORIDE
3,5,7-Triaza-1-azoniaadamantane, 1-(2-thienyl)-, chloride
Hexamethylenetetramine, compd. with thiophene, 2-(chloromethyl)-
6296-08-8

Properties Computed from Structure:

Molecular Weight: 272.79748 g/mol
Molecular Formula: $C_{11}H_{17}ClN_4S$
Hydrogen Bond Donor Count: 0
Hydrogen Bond Acceptor Count: 4
Rotatable Bond Count: 2
Topological Polar Surface Area: 9.7
more...

Descriptors Computed from Structure:

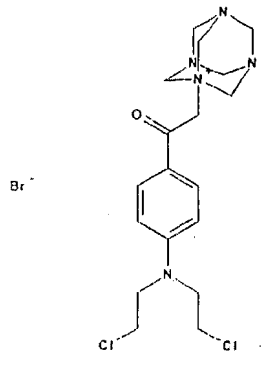
Canonical SMILES: C1N2CN3CN1C[N+](C2)(C3)CC4=CC=CS4.[Cl-]
InChI: InChI=1/C11H17N4S.ClH/c1-2-11(16-3-1)4-15-8-12-5-13(9-15)7-14(6-12)10-15;/h1-3H,4-10H2;1H/q+1;/p-1/fC11H17N4S.Cl/h;1h/qm;-1

Substance Category:

Biological Properties: 2 Links
Toxicology: 1 Link

ASN1	Display / Save	XML	Display / Save	SDF	Display / Save

Compound Summary:



CID: 64172
Parent CID: 64173
Unique Components: 2 Links

NLM Toxicology: Link
Substances: 2 Links
Similar Compounds: 2 Links
Structure Search

MeSH | Synonyms | Properties | Descriptors | Category | Exports

Medical Subject Annotations: (Total:1)

AT 584

PubMed via MeSH

PubMed MeSH Keyword Summary

Depositor-Supplied Synonyms: (Total: 9)

Sort: Weight

AT 584
AT-584
1-(p-(Bis(2-chloroethyl)amino)phenacyl)-3,5,7-triaza-1-azoniaadamantane bromide
3,5,7-Triaza-1-azoniaadamantane, 1-(p-(bis(2-chloroethyl)amino)phenacyl)-, bromide
Hexamethylenetetramine salt of p-(bis(2-chloroethyl)amino)-alpha-bromoacetophenone
1-(2-(4-(Bis(2-chloroethyl)amino)phenyl)-2-oxoethyl)-3,5,7-triaza-1-azoniatricyclo(3.3.1.1(sup 3,7))decane bromide
16810-17-6
3,5,7-Triaza-1-azoniatricyclo(3.3.1.1(sup 3,7))decane, 1-(2-(4-(bis(2-chloroethyl)amino)phenyl)-2-oxoethyl)-, bromide
3.5,7-Triaza-1-azoniatricyclo(3.3.1.13,7)decane, 1-(2-(4-(bis(2-chloroethyl)amino)phenyl)-2-oxoethyl)-, bromide

Properties Computed from Structure:

Molecular Weight: 479.24194 g/mol
Molecular Formula: $C_{18}H_{26}BrCl_2N_5O$
Hydrogen Bond Donor Count: 0
Hydrogen Bond Acceptor Count: 6
Rotatable Bond Count: 8
Tautomer Count: 2
Topological Polar Surface Area: 30
more...

Descriptors Computed from Structure:

Canonical SMILES: C1N2CN3CN1C[N+](C2)(C3)CC(=O)C4=CC=C(C=C4)N(CCCl)CCCl.[Br-]
InChI: InChI=1/C18H26Cl2N5O.BrH/c19-5-7-24(8-6-20)17-3-1-16(2-4-17)18(26)9-25-13-21-10-22(14-25)12-23(11-21)15-25;/h1-4H,5-15H2;1H/q+1;/p-1/fC18H26Cl2N5O.Br/h;1h/qm;-1

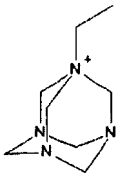
Substance Category:

Biological Properties: 1 Link

Toxicology: 1 Link

ASN1	Display Save	**XML**	Display Save	**SDF**	Display Save

Compound Summary:



CID: 64160

BioActivity: Summary
Inactive: 2 Links

Substances:
All: 7 Links
Same: 5 Links
Mixture: 2 Links

Similar Compounds: 5 Links

Structure Search

Synonyms | Properties | Descriptors | Category | Exports

Depositor-Supplied Synonyms: (Total: 16)

Display: First 10 | All, | Sort: Weight

Formoiodine
Hexamethylenetetramine ethyl-
Hexamethylenetetramine ethyl iodide

NSC7308
NSC7308 (IODINE SALT)
AIDS155858
AIDS-155858
NSC203331
5406-76-8 (IODDINE SALT)
3,5, 7-Triaza-1-azoniaadamantane, 1-ethyl-
3,5, 7-Triaza-1-azoniaadamantane, 1-ethyl-, iodide
1-Ethyl-1lambda~5~,3,5,7-tetraazatricyclo[3.3.1.1~3,7~]decane
3,5, 7-Triaza-1-azoniatricyclo[3.3.1.13,7]decane, 1-ethyl-
3,5, {7-Triaza-1-azoniatricyclo[3.3.1.13,7]decane,} 1-ethyl-, iodide
3,5, 7-Triaza-1-azoniatricyclo[3.3.1.13,7]decane, 1-ethyl-, iodide
5406-76-8

Properties Computed from Structure:

Molecular Weight: 169.24738 g/mol
Molecular Formula: $C_8H_{17}N_4^+$
Hydrogen Bond Donor Count: 0
Hydrogen Bond Acceptor Count: 3
Rotatable Bond Count: 1
Topological Polar Surface Area: 9.7
more...

Descriptors Computed from Structure:

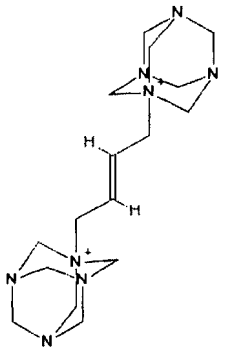
Canonical SMILES: CC[N+]12CN3CN(C1)CN(C3)C2
InChI: InChI=1/C8H17N4/c1-2-12-6-9-3-10(7-12)5-11(4-9)8-12/h2-8H2,1H3/q+1

Substance Category:

Biological Properties: 4 Links
Theoretical Properties: 1 Link

ASN1	Display / Save	XML	Display / Save	SDF	Display / Save

Compound Summary:



CID: 6435994
Parent CID: 6435995
Unique Components: 2 Links

NLM Toxicology: Link
Substance: 1 Link
Similar Compounds: 2 Links
Structure Search

Synonyms | Properties | Descriptors | Category | Exports

Depositor-Supplied Synonyms: (Total: 10)

Sort: Weight

Cosan 265
Caswell No. 259AA
EINECS 257-149-1

EPA Pesticide Chemical Code 106801
1,1'-(2-Butylene)bis(3,5,7-triaza-1-azoniaadamantane)
1,1'-(2-Butenylene)bis(3,5,7-triaza-1-azoniaadamantane chloride
1,1'-(But-2-en-1,4-diyl)bis(3,5,7-triaza-1-azoniatricyclo(3.3.1.13,7)decane) dichloride
3,5,7-Triaza-1-azoniatricyclo(3.3.1.13,7)decane, 1,1'-(2-butene-1,4-diyl)bis-, dichloride
51350-84-6
59736-58-2

Properties Computed from Structure:

Molecular Weight: 405.369 g/mol
Molecular Formula: $C_{16}H_{30}Cl_2N_8$
Hydrogen Bond Donor Count: 0
Hydrogen Bond Acceptor Count: 8
Rotatable Bond Count: 4
Topological Polar Surface Area: 19.4
more...

Descriptors Computed from Structure:

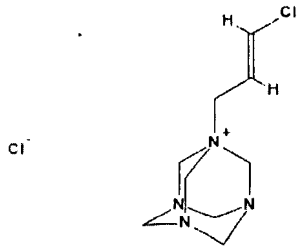
Canonical SMILES: C1N2CN3CN1C[N+](C2)(C3)CC=CC[N+]45CN6CN(C4)CN(C6)C5.[Cl-].[Cl-]
Isomeric SMILES: C1N2CN3CN1C[N+](C2)(C3)C\C=C\C[N+]45CN6CN(C4)CN(C6)C5.[Cl-].[Cl-]
InChI: InChI=1/C16H30N8.2ClH/c1(3-23-11-17-5-18(12-23)7-19(6-17)13-23)2-4-24-14-20-8-21(15-24)10-22(9-20)16-24;;/h1-2H,3-16H2;2*1H/q+2;;/p-2/b2-1+;;/fC16H30N8.2Cl/h;2*1h/qm;2*-1

Substance Category:

Toxicology: 1 Link

ASN1	Display / Save	XML	Display / Save	SDF	Display / Save

Compound Summary:



CID: 6433396
Parent CID: 5475987
Unique Components: 2 Links

NLM Toxicology: Link

Substances: 3 Links

Related Compounds:
Same, Connectivity: 2 Links

Similar Compounds: 11 Links

Structure Search

MeSH | Synonyms | Properties | Descriptors | Category | Exports

Medical Subject Annotations: (Total:1)

quaternium-15

PubMed via MeSH

PubMed MeSH Keyword Summary

Depositor-Supplied Synonyms: (Total: 24)

Display: First 10 | All | Sort: Weight

Dowicide Q
Quaternium 15
Quaternium-15
Dowicil 75
Cinartc 200
Dowicil 100
Caswell No. 181
Dowco 184
CCRIS 1398
HSDB 6820
Methenamine 3-chloroallylochloride
EINECS 223-805-0
N-(3-Chloroallyl)hexaminium chloride
EPA Pesticide Chemical Code 017901
NSC 172971
XD-1840
Hexamethylenetetramine chloroallyl chloride
N-(3-CHLORALLYL)HEXAMINIUM CHLORIDE
1-(3-Chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride
3,5,7-Triaza-1-azoniaadamantane, 1-(3-chloroallyl)-, chloride
3,5,7-Triaza-1-azoniatricyclo(3.3.1.13,7)decane, 1-(3-chloro-2-propenyl)-, chloride
103638-29-5
4080-31-3
60789-82-4

Properties Computed from Structure:

Molecular Weight: 251.15614 g/mol
Molecular Formula: $C_9H_{16}Cl_2N_4$
Hydrogen Bond Donor Count: 0
Hydrogen Bond Acceptor Count: 4
Rotatable Bond Count: 2
Topological Polar Surface Area: 9.7
more...

Descriptors Computed from Structure:

Canonical SMILES: C1N2CN3CN1C[N+](C2)(C3)CC=CCl.[Cl-]
Isomeric SMILES: C1N2CN3CN1C[N+](C2)(C3)C\C=C\Cl.[Cl-]
InChI: InChI=1/C9H16ClN4.ClH/c10-2-1-3-14-7-11-4-12(8-14)6-13(5-11)9-14;/h1-2H,3-9H2;1H/q+1;/p-1/b2-1+;/fC9H16ClN4.Cl/h;1h/qm;-1

Substance Category:

Biological Properties: 1 Link
Journal Publishers: 1 Link
Toxicology: 1 Link

ASN1	Display / Save	**XML**	Display / Save	**SDF**	Display / Save